Crossover from adiabatic to antiadiabatic quantum pumping with dissipation

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Quantum pumping, in its different forms, is attracting attention from different fields, from fundamental quantum mechanics, to nanotechnology, to superconductivity. We investigate the crossover of quantum pumping from the adiabatic to the anti-adiabatic regime in the presence of dissipation, and find general and explicit analytical expressions for the pumped current in a minimal model describing a system with the topology of a ring forced by a periodic modulation of frequency ω. The solution allows following in a transparent way the evolution of pumped DC current from much smaller to much larger ω values than the other relevant energy scale, the energy splitting introduced by the modulation. We find and characterize a temperature-dependent optimal value of the frequency for which the pumped current is maximal.

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A current with a net DC component can be pumped in an electronic system without leads and bias voltages, through a "peristaltic" modulation of the transmission amplitudes and gate voltages [1]. This effect has both classical and quantum components [2, 3], and occurs for unpaired electrons as well as for Cooper pairs [4, 5]. When the modulation is adiabatic i.e., when the pumping period is much longer than the intrinsic time-scale of the system, so that transitions between states do not occur, it has long been recognized that the charge pumped over a period has a geometric nature [2, 3, 6] and is in many cases quantized. These geometrical aspects survive even in the presence of a coupling between the electrons and an external phonon bath, despite the obvious source of inelastic effects represented by the bath [4, 5, 7]. Unsurprisingly, like in classical pumps, the current in this slow, adiabatic regime increases proportionally to the driving frequency $\omega/2\pi$, as long as $\hbar\omega$ is much smaller than all intrinsic energy scales of the system.

The question we address in this Letter is: of what kind, and of what magnitude are the deviations from adiabatic pumping that will show up in the DC current when the pumping frequency grows higher and higher? What is the behavior of the DC current as frequency crosses over beyond the adiabatic and into the antiadiabatic ($\omega \to \infty$) regime? To obtain specific answers, we shall focus on the crossover from adiabatic to antiadiabatic quantum pumping (or "stirring" [3, 8, 9]) in a system with the topology of a ring, in the presence of dissipation. For a particular but reasonable choice of coupling to the bath, we find that the dissipative model admits a full analytical solution for the steady state current valid at arbitrary frequency. Through that solution we can analyze and understand the main predicted features of pumping-frequency dependence of the DC current. At low frequencies the pumped current tracks the known adiabatic result, namely DC current increases linearly with frequency, and the pumped charge is as expected geometric in nature (albeit not quantized). However, and this is a surprising outcome, the pumped DC current turns non-monotonic for increasing ω, going through a temperature-dependent optimal value and then dropping eventually as ω^{-1} for $\omega \to \infty$. Beyond the strict limits of the present model, we also surmise that these results are representative of a larger class of orbital doublet systems weakly coupled to a generic environment.

Consider the minimal model constituted by a three-site ring as in Fig. 1, each of the identical sites a, b, c endowed with a single nondegenerate electronic level of energy $\epsilon_i(t)$, and different sites coupled by hoppings $\gamma_{ij}(t)$, where $i, j = a, b, c$. Current pumping can be obtained, for instance, by letting $\gamma_{ij} = \gamma_0$ and externally actuating a cyclic variation of the three on-site energies $\epsilon_i(t) = -\hbar\Delta\cos(\omega t + \phi_i)$, with $\phi_a = 0$, $\phi_b = -2\pi/3$, $\phi_c = +2\pi/3$. In the perturbative limit ($\hbar\Delta \ll \gamma_0$) the three-site ring can be replaced by a simpler effective orbital pseudospin model obtained by removing the totally symmetric state $|0\rangle = (|a\rangle + |b\rangle + |c\rangle)/\sqrt{3}$ (of energy $-2\gamma_0$ for $\Delta = 0$, doubly occupied and irrelevant) to retain only the two states $|x\rangle = (|b\rangle - |c\rangle)/\sqrt{2}$, and $|y\rangle = (2|a\rangle - |b\rangle - |c\rangle)/\sqrt{6}$, orbitally degenerate in the unperturbed ring $\Delta = 0$, with energy γ_0. The single mobile electron now occupies the orbital doublet $|x\rangle$, $|y\rangle$, leading to a pseudospin-1/2 problem with the time-dependent

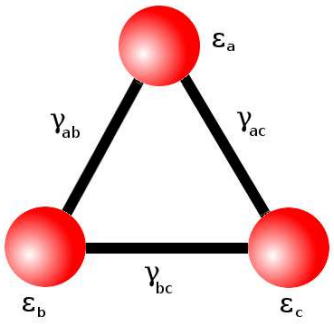

FIG. 1: Schematic of the minimal ring model, realized by three quantum-dots a, b, c with externally controlled potentials ϵ_a, ϵ_b and ϵ_c used for pumping. The γ_{ij} are here inter-dot hoppings, generally fixed. An alternative realization could be a molecular trimer [10, 11] where three atomic orbitals $|a\rangle$, $|b\rangle$ and $|c\rangle$ have identical energies, while the hopping integrals γ_{ij} can actuate the pumping by modulating atomic displacements. In either case the relevant states of the system can be mapped to the pseudospin-1/2 model of Eq. (1).

Hamiltonian [12]:

$$\mathcal{H}_S(t) = \frac{\hbar\Delta}{2}\left[\cos(\omega t)\sigma^z + \sin(\omega t)\sigma^x\right] , \qquad (1)$$

where σ^ξ are Pauli matrices. The current $I(t) = \langle I_{ab}\rangle = -iq_e\gamma_0\langle c_b^\dagger c_a - c_a^\dagger c_b\rangle$ (where q_e is the elementary charge) in the pseudospin representation is given by $I(t) = I_0\langle\sigma^y\rangle$, where $I_0 = q_e\gamma_0/\sqrt{3}$.

While this is the same type of Hamiltonian previously used to study adiabatic pumping [4], we now find that this problem allows a more general analytical solution for arbitrary pumping frequency beyond the adiabatic regime, and in the presence of a coupled bath, so long as the coupling is weak. The exact time evolution induced by (1) can be obtained by noting that $H = (\hbar\Delta/2)R_y(\omega t)\sigma_z R_y^{-1}(\omega t)$, where $R_y(\omega t) = e^{-i\omega t\sigma^y/2}$, represents a uniform rotation by an angle ωt around the y-axis. Performing this time-dependent unitary transformation and defining $|\psi(t)\rangle = R_y(\omega t)|\tilde\psi(t)\rangle$, the Schrödinger equation for $|\tilde\psi\rangle$ is governed by the effective Hamiltonian

$$\mathcal{H}_{\rm eff} = R_y^{-1}\mathcal{H}_S R_y - iR_y^{-1}\dot R_y = \frac{\hbar}{2}\left(\Delta\sigma^z - \omega\sigma^y\right) = \frac{\hbar\omega'}{2}\hat{\mathbf{n}}\cdot\boldsymbol{\sigma} .$$

This now represents a time-independent field pointing in the direction $\hat{\mathbf{n}} = (0, -\omega/\omega', \Delta/\omega')$, where $\omega' = \sqrt{\omega^2+\Delta^2}$ is the associated Larmor frequency. The problem thus has a simple solution in this reference frame: the spin state $|\tilde\psi\rangle$ precesses around $\hat{\mathbf{n}}$, while the current retains the form $I(t) = I_0\langle\tilde\psi(t)|\sigma^y|\tilde\psi(t)\rangle$. The current carried by the eigenstates $|\hat{\mathbf{n}};\pm\rangle$ of $\mathcal{H}_{\rm eff}$ is $I_0\langle\mathbf{n};\pm|\sigma^y|\hat{\mathbf{n}};\pm\rangle = \mp I_0\omega/\omega'$, respectively. In the absence of coupling to the bath, all time dependence of the current is determined just by the initial conditions. In particular, the two eigenvectors of $\mathcal{H}_{\rm eff}$ carry a pure (and opposite) DC current, while any other initial condition yields a DC plus an AC current. The DC component is determined by the projection of the pseudospin onto the eigenstates of $\mathcal{H}_{\rm eff}$:

$$I = I_0\, P\, \frac{\omega}{\omega'} , \qquad (2)$$

with the pseudospin polarization $P = -{\rm Tr}(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}\,\tilde\rho_S)$ expressed in terms of the density matrix operator $\tilde\rho_S$ in the rotating frame.

Even if one prepares the initial density matrix in a pure state, the slightest dissipation will eventually drive the system to a different (generally periodically time-dependent) steady state. To describe the effect of dissipation, we introduce the environment in the standard form [13] of a heat bath of harmonic oscillators at temperature T linearly coupled to the charge fluctuations, embodied in this system by the two operators σ_z and σ_x. The dissipative part of the Hamiltonian is thus $\mathcal{H}_B + \mathcal{H}_{SB}$ where:

$$\mathcal{H}_B = \sum_{\xi=z,x}\sum_\nu\left[\frac{p_{\xi,\nu}^2}{2m} + \frac{m\omega_\nu^2 q_{\xi,\nu}^2}{2}\right] , \qquad (3)$$

$$\mathcal{H}_{SB} = \sum_{\xi=z,x}\sum_\nu\sqrt{\frac{2m\omega_\nu}{\hbar}}\lambda_{\xi,\nu}q_{\xi,\nu}\sigma^\xi . \qquad (4)$$

Here ω_ν are the oscillator frequencies and $\lambda_{\xi,\nu}$ are coupling constants, for which we assume ohmic spectral densities [13, 14] $J_\xi(\omega) = \sum_\nu \lambda_{\xi,\nu}^2\delta(\omega-\omega_\nu) = \hbar^2\alpha_\xi\omega e^{-\omega/\omega_c}$.

Assuming the coupling to be weak, $\alpha_\xi \ll 1$, and retaining the lowest-order in α_ξ, the evolution of the system's reduced density matrix $\tilde\rho_S$ in the rotating frame is given by the master equation [15]

$$\frac{\partial\tilde\rho_S(t)}{\partial t} \simeq -i[\mathcal{H}_{\rm eff},\tilde\rho_S(t)] - \frac{1}{\hbar^2}\sum_{\xi=z,x}\int_0^\infty d\tau \qquad (5)$$
$$\Big\{G_\xi(\tau)\left[\tilde\sigma^\xi(t), U_0^\dagger(-\tau)\tilde\sigma^\xi(t-\tau)U_0(-\tau)\tilde\rho_S(t)\right]$$
$$+ G_\xi^*(\tau)\left[\tilde\rho_S(t)U_0^\dagger(-\tau)\tilde\sigma^\xi(t-\tau)U_0(-\tau), \tilde\sigma^\xi(t)\right]\Big\} ,$$

where $\tilde\sigma^\xi(t) = R_y^{-1}(\omega t)\sigma^\xi R_y(\omega t)$, and $U_0(\tau) = \exp(-i\mathcal{H}_{\rm eff}\tau/\hbar)$. The function $G_\xi(\tau)$ is expressed in terms of the spectral density as

$$G_\xi(\tau) = \int_0^\infty d\omega J_\xi(\omega)\left[\cos(\omega\tau)\coth\frac{\hbar\omega\beta}{2} - i\sin(\omega\tau)\right] ,$$

where $\beta = (k_{\rm B}T)^{-1}$, and T is the bath temperature.

When the bath coupling to σ_x and σ_z have the same spectral density ($J_x(\omega) = J_z(\omega) = J(\omega)$, even if non-ohmic) the form of Eq. (5) becomes particularly simple, since all explicit time dependence disappears and we are left with a constant-coefficients inhomogeneous linear differential equation [12]. For $\alpha_\xi \to 0$ we find that the stationary density matrix $\tilde\rho_S$ is diagonal in the basis $|\mathbf{n}\pm\rangle$,

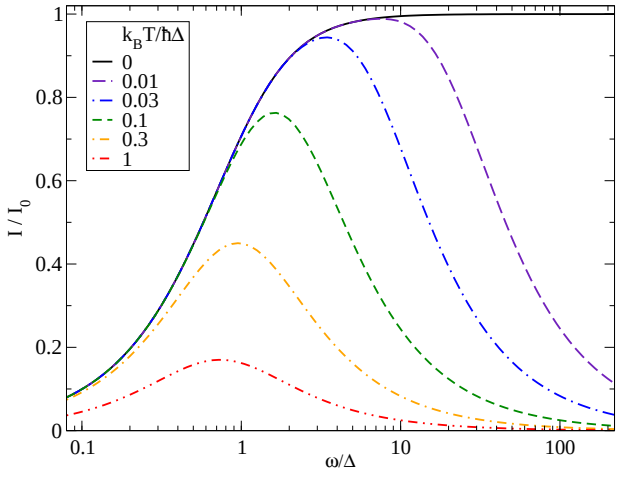

FIG. 2: Steady-state DC circulating current I as a function of the pumping frequency ω. Solid line: $T = 0$ current, obtained by Eq. (2) with $P \equiv 1$. Note that this coincides with the purely quantum result (no dissipation) when $|\tilde{\psi}\rangle = |\hat{\mathbf{n}}; -\rangle$ is chosen for the initial state. Dashed and dot-dashed curves: pumped DC current for several temperatures, as obtained by the exact expression (6) for P.

with a polarization given by

$$P = \frac{(\omega' - \omega)^2 J_+ + (\omega' + \omega)^2 J_-}{(\omega' - \omega)^2 c_+ J_+ + (\omega' + \omega)^2 c_- J_-} \,. \qquad (6)$$

Here $J_\pm = J(\omega' \pm \omega)$ and $c_\pm = \coth[\hbar(\omega' \pm \omega)/(2k_{\rm B}T)]$. The resulting DC circulating current, Eq. (2), is shown in Fig. 2 for a broad range of frequency and temperature.

Several comments are in order. (i) In the $T \to 0$ limit, irrespective of ω/Δ and of the form of the spectral density, the stationary master equation operator is a projector onto the ground state $|\mathbf{n}-\rangle$ of $\mathcal{H}_{\rm eff}$. (ii) For $\omega \ll \Delta$, we have $P = \tanh[\hbar\Delta/(2k_{\rm B}T)]$ as is appropriate for a static Hamiltonian in thermal equilibrium. At $T = 0$, $P = 1$ and the charge pumped in a period, $Q_p = 2\pi I/\omega = 2\pi I_0/(\hbar\Delta)$ coincides exactly with the Berry-phase result [16] of Eq. (21) in Ref. [6]. Nevertheless, the pumped charge, although geometric, is not quantized, and depends on the ratio γ_0/Δ. It can be made quite large (though not arbitrarily large) by reducing the amplitude of the perturbing field Δ in the range $\hbar\omega \ll \hbar\Delta \ll \gamma_0$. (iii) Finally, in the antiadiabatic regime $\omega \gg \Delta$ we find $P = \tanh[\hbar(\omega' - \omega)/(2k_B T)]$. This result is at first sight intriguing: for fast driving, the spin reaches thermal equilibrium like a static spin Hamiltonian characterized by an effective Larmor frequency $(\omega' - \omega) = \Delta[\Delta/(2\omega) + O(\Delta/\omega)^3]$ that vanishes for large ω. The polarization, which remains identically unity for all large frequencies at $T = 0$, decays eventually at any finite T for large ω. Faster and faster driving at finite temperature enhances the pumped current up to $\omega \simeq \hbar\Delta^2/k_B T$. For larger driving frequencies, thermal fluctuations catch up and suppress P causing the pumped current I to drop, as seen on the high-frequency side of Fig. 2. The reason why $(\omega' - \omega)$ determines the Boltzmann occupancy of the two levels split by $\hbar\omega'$ may be traced to the $-\omega \cdot \mathbf{M}$ term to be included in the thermodynamically relevant functions for a body rotating at frequency ω, see e.g., §26 of Ref. [17], where $\mathbf{M}$ is the body angular momentum which, for our spin, coincides with $\hbar\boldsymbol{\sigma}$.

The results just presented are analytical and thus quite elegant and predictive. Obtained as they were for a rather special case however, how general are they? To address this question we solve numerically Eq. (5) by means of Runge-Kutta integration [18], and obtain $\tilde{\rho}_S(t)$ and from that $I(t) = I_0 {\rm Tr}[\sigma^y \tilde{\rho}_S(t)]$. The numerical approach allows us to study the effect of unequal environments in the x and z directions, where the simplifications leading to Eq. (6) do not hold. In particular, we consider the case $\alpha_x \neq \alpha_z$ (by symmetry, it does not matter which one is larger). We find that at finite (but small) α_ξ the solution is no longer stationary even in the rotating reference frame chosen, and small oscillations of the density matrix and of the current at frequency 2ω remain undamped in the long-time limit. Nevertheless for $\alpha_\xi \to 0$, the amplitude of these oscillating density-matrix terms vanishes linearly with α_ξ, and the constant part of the density matrix at low temperature converges to the symmetric-environment case. In particular, at $T = 0$ the polarization again saturates to 1.

This behavior for $\alpha_\xi \to 0$ can alternatively be recovered by applying a rotating wave approximation to Eq. (5), i.e., by neglecting all the terms oscillating with frequency ω or ω'. Remarkably, the resulting equation again coincides without approximations with the one appropriate to the symmetric environment. We conclude that the results obtained for the symmetric environment are indeed representative of those expected in the more general asymmetric coupling case, provided the limit of weak coupling to the environment holds. In particular, Eq. (6) remains valid.

The numerical solution of the master equation (5) also illustrates the transient approach to the stationary state. Figure 3 shows the full time evolution of the current, compared to the pure quantum evolution in the absence of dissipation. Note that, for a given coupling α, temperature affects not only the final steady current, via the final value of P, see Eq. (6) and inset of Fig. 3, but also the relaxation time with which this steady state is approached in the initial transient.

In Ref. [4] an investigation was attempted of nonadiabaticity, with numerical evidence that a stronger dissipation might somehow compensate for the weak-coupling non-adiabatic current reduction relative to the geometric value of the adiabatic limit. Our exact solution clarifies that nonadiabaticity is fundamentally associated to such a radical current suppression that eventually, for large frequency, the charge pumped in one period $Q_p \propto \omega^{-2}$.

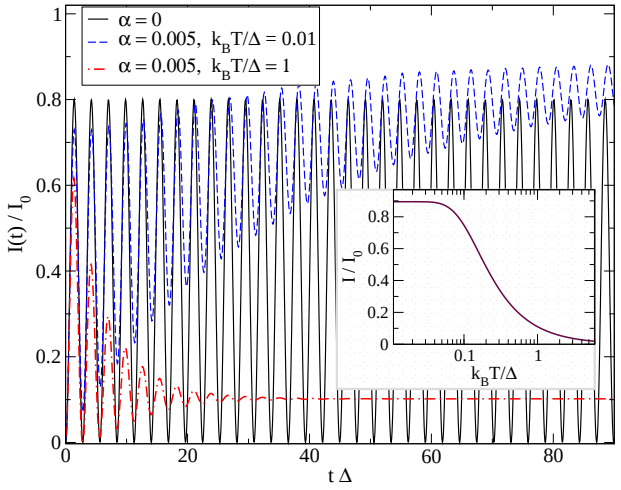

FIG. 3: Time evolution of the current $I(t) = I_0 \mathrm{Tr}[\sigma^y \tilde{\rho}_S(t)]$ for $\omega = 2\Delta$, in the dissipationless case ($\alpha = 0$, solid curve), and in the transient induced by weak dissipation ($\alpha = 0.005$), at low (dashed) and intermediate temperature (dot-dashed), starting from the initial $|z, -\rangle$ state. Inset: temperature dependence of the steady-state dc current I.

The method introduced in a very recent work [5] also can deal with the non-adiabatic regime (indeed our $|\mathbf{n}\pm\rangle$ states coincide with the Floquet states of that method), and represents a more general approach to pumping problems in the presence of weak dissipation [19]. However in that work intermediate frequencies were studied only in the absence of dissipation: the present model seems unique in affording an explicit analytic expression for the density matrix and current in the presence of dissipation for arbitrarily high frequency.

Feasibility and quantitative estimates – Triple quantum dot systems have been recently realized experimentally [20], and could be used to implement the pumping effect proposed. By adopting a tentative hopping $\gamma_0 \simeq 0.05$ meV between the dots, we find a maximum current of the order of $I_0 = 0.05\ \mathrm{meV}\, q_e/(\sqrt{3}\hbar) \simeq 7$ nA. The magnetic field generated by this current could be detectable if the dot-ring arrangement had at least an effective radius $r_{\rm eff} \simeq 200$ nm [21]. In that case, a ring-shaped SQUID of $5\,\mu$m radius placed $\sim 5\,\mu$m above the quantum dots would intercept a flux of order 0.02 flux quanta, a value routinely detectable.

The frequency and temperature regions where this current enhancement could be detected are determined by the frequency scale Δ of the effective spin-1/2 model. Assuming $\Delta \simeq 0.1\gamma_0/\hbar \simeq 8$ GHz, the predicted frequency-dependent dissipative effects on current should be observed near and mainly above this resonant angular frequency at temperature $T \lesssim 0.2\hbar\Delta/k_{\rm B}$, i.e., about $T \lesssim 0.01$ K for the three-dot setup. Our model could be relevant in a molecular context as well, where an electronically degenerate point is looped about, as for example due to cyclic molecular distortions, see Fig. 1 and Ref. [12].

In summary, we presented an analytical solution for the time-dependent pumping of DC current in a quantum model with dissipation, valid in the weak dissipation limit. The solution fully covers the crossover from the well-known adiabatic limit to arbitrarily high frequencies. The main physical surprise is that the frequency dependence of current is nonmonotonic, with an optimal value that moves from Δ upwards to infinity as temperature is reduced. This effect, on the whole reminiscent of magnetic-resonance physics, could be directly detectable for example in multi-dot arrangements.

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